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The Incremental and Differential Maxwell Garnett Formalisms for Bianisotropic Composites

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Abstract

We present two approaches to homogenize bianisotropic particulate composite mediums: (i) the Incremental Maxwell Garnett (IMG) formalism, in which the composite medium is built incrementally by adding the inclusions in N discrete steps to the host medium; and (ii) the Differential Maxwell Garnett (DMG) formalism, which is obtained from the IMG in the limit $N \to \infty$. Both formalisms are applicable to arbitrary inclusion concentration and are well–suited for computational purposes. Application of both formalisms is exemplified here by numerical results for a uniaxial dielectric composite medium and a chiroferrite.

1. Introduction

Discrete random mediums — comprising electrically small particles of a certain material dispersed randomly in some host medium — have been considered in the electromagnetics literature for about two centuries as homogeneous material continuums. Several homogenization formalisms exist to connect the electromagnetic response properties of a homogenized composite medium (HCM) to those of the constituent material phases; see Ref. [1] for a selection of milestone papers about this topic.

Perhaps the most widely used homogenization formalism is the Maxwell Garnett (MG) formalism. It was recently set up for bianisotropic composite mediums containing ellipsoidal inclusions [2], [3], covering thereby a large domain of electromagnetic applications in the materials sciences. One drawback of the MG formalism is that it can be used only for dilute composite mediums.

Our present work illustrates and enlarges upon an earlier report [4] on overcoming this handicap of the MG formalism. The so–called Incremental Maxwell Garnett (IMG) formalism is applicable to dense composite mediums. It has an iterative flavour, being based on the repeated use of the MG formalism for certain *intermediate* dilute composite mediums. Furthermore, we show that the IMG formalism leads to a Differential Maxwell Garnett (DMG) formalism that is based on the numerical solution of a system of differential equations. Details of the IMG/DMG formalisms shall be published shortly elsewhere [5]. A more general survey of homogenization formalisms for bianisotropic composite mediums is given in Ref. [6]; see also Ref. [7].

2. Theory

Suppose that identical, similarly oriented, electrically small inclusions made of a medium labelled b are randomly dispersed in a host medium labelled a. The volumetric proportions of the constituent material phases are denoted by f_a and $f_b = 1 - f_a$. Both mediums are linear and bianisotropic, their frequency–domain constitutive relations being specified as [3], [4]:

$$\begin{pmatrix} \underline{D} \\ \underline{B} \end{pmatrix} = \underline{\underline{\mathbf{C}}}^{\alpha} \cdot \begin{pmatrix} \underline{E} \\ \underline{H} \end{pmatrix}, \qquad (\alpha = \mathrm{a},\, \mathrm{b})\,. \tag{1}$$

The 6×6 constitutive dyadic $\underline{\underline{\mathbf{C}}}^{\alpha}$ is composed of 3 × 3 dyadics in the following way:

$$\underline{\underline{\mathbf{C}}}^{\alpha} = \begin{pmatrix} \underline{\underline{\epsilon}}^{\alpha} & \underline{\underline{\xi}}^{\alpha} \\ \underline{\underline{\zeta}}^{\alpha} & \underline{\underline{\mu}}^{\alpha} \end{pmatrix}, \qquad (\alpha = \mathrm{a},\, \mathrm{b})\,, \tag{2}$$

where $\underline{\underline{\epsilon}}^{\alpha}$ and $\underline{\underline{\mu}}^{\alpha}$ are the permittivity and permeability dyadics, respectively, whereas $\underline{\underline{\xi}}^{\alpha}$ and $\underline{\underline{\zeta}}^{\alpha}$ are the two magnetoelectric dyadics. An $\exp(-i\omega t)$ time–dependence is implicit in this work, ω being the angular frequency.

We define the 6×6 polarizability dyadic

$$\underline{\underline{\mathbf{a}}}^{\alpha' \,\mathrm{in}\, \alpha} = \left(\underline{\underline{\mathbf{C}}}^{\alpha'} - \underline{\underline{\mathbf{C}}}^{\alpha}\right) \cdot \left[\underline{\underline{\mathbf{I}}} + i\omega \underline{\underline{\mathbf{D}}}^{\alpha} \cdot \left(\underline{\underline{\mathbf{C}}}^{\alpha'} - \underline{\underline{\mathbf{C}}}^{\alpha}\right)\right]^{-1} \tag{3}$$

of an electrically small ellipsoid of medium α' embedded *in* medium α, where $\underline{\underline{\mathbf{I}}}$ is the 6×6 identity dyadic. In the general case of a bianisotropic medium, the 6×6 depolarization dyadic $\underline{\underline{\mathbf{D}}}^{\alpha}$ can be computed by numerical two–dimensional integration, and in many important cases even analytically [6].

The MG estimate $\underline{\underline{\mathbf{C}}}^{\mathrm{MG}}$ of the constitutive dyadic of the HCM is given by [2]

$$\underline{\underline{\mathbf{C}}}^{\mathrm{MG}}(\underline{\underline{\mathbf{C}}}^{\mathrm{a}}, \underline{\underline{\mathbf{C}}}^{\mathrm{b}}, f_{\mathrm{b}}) = \underline{\underline{\mathbf{C}}}^{\mathrm{a}} + f_{\mathrm{b}}\, \underline{\underline{\mathbf{a}}}^{\mathrm{b\,in\,a}} \cdot \left(\underline{\underline{\mathbf{I}}} - i\omega f_{\mathrm{b}}\, \underline{\underline{\tilde{\mathbf{D}}}}^{\mathrm{a}} \cdot \underline{\underline{\mathbf{a}}}^{\mathrm{b\,in\,a}}\right)^{-1}, \tag{4}$$

where $\underline{\underline{\tilde{\mathbf{D}}}}^{\alpha}$ is related to $\underline{\underline{\mathbf{D}}}^{\alpha}$ and the functional dependencies of $\underline{\underline{\mathbf{C}}}^{\mathrm{MG}}$ are identified explicitly.

In the *IMG formalism*, the actual composite medium is built *incrementally* by adding the inclusions not all at once, but in N stages. After each increment, the composite medium is homogenized using the MG formalism. In this fashion, the following iterative scheme emerges

$$\underline{\underline{\mathbf{C}}}^{(0)} = \underline{\underline{\mathbf{C}}}^{\mathrm{a}}, \qquad \underline{\underline{\mathbf{C}}}^{(\mathrm{n}+1)} = \underline{\underline{\mathbf{C}}}^{\mathrm{MG}}(\underline{\underline{\mathbf{C}}}^{(\mathrm{n})}, \underline{\underline{\mathbf{C}}}^{\mathrm{b}}, \delta_{\mathrm{b}}), \qquad (n = 0,\, 1,\, 2, \ldots)\,. \tag{5}$$

In order to terminate the iterative scheme in N stages, we fix the incremental proportion

$$\delta_{\mathrm{b}} = 1 - (1 - f_{\mathrm{b}})^{1/N}\,. \tag{6}$$

As the final result of the iteration, we obtain the IMG estimate $\underline{\underline{\mathbf{C}}}^{\mathrm{IMG}} = \underline{\underline{\mathbf{C}}}^{(\mathrm{N})}$.

The *DMG formalism* arises from the IMG formalism in the limit $N \to \infty$. The difference equation (5) is then converted into the ordinary differential equation

$$\frac{\partial}{\partial \eta} \underline{\underline{\mathbf{C}}}(\eta) = \frac{1}{1-\eta} \underline{\underline{\mathbf{a}}}^{\mathrm{b\,in}\,\eta}, \tag{7}$$

with initial value $\underline{\underline{\mathbf{C}}}(0) = \underline{\underline{\mathbf{C}}}^{\mathrm{a}}$. The DMG estimate is then given by

$$\underline{\underline{\mathbf{C}}}^{\mathrm{DMG}} = \underline{\underline{\mathbf{C}}}(f_{\mathrm{b}})\,. \tag{8}$$

3. Numerical Results and Discussion

Two independent numerical implementations of the IMG and DMG formalisms were set up by us. Both codes produced identical results in all cases tested. The number of iteration steps for the IMG formalism is finite, because N is finite, and therefore no convergence problems can arise so long as an adequately large value of N is used [4]. For implementing the DMG formalism, one can rely on well–tested algorithms in numerical libraries so that no numerical problems are to be expected either. Thus, the IMG and DMG implementations are more robust than the implementation of the Bruggeman (Br) formalism.

We now illustrate the IMG and DMG formalisms in relation to the MG and Br formalisms and begin with the simple case of a composite medium consisting of a uniaxial dielectric host medium with spherical isotropic dielectric inclusions. That is,

$$\underline{\underline{\epsilon}}^{\mathrm{a}} = \epsilon_0 \left(\underline{\underline{I}} + 3\, \underline{u}\, \underline{u} \right) , \quad \underline{\underline{\epsilon}}^{\mathrm{b}} = 10\, \epsilon_0\, \underline{\underline{I}} ; \quad \underline{\underline{\mu}}^{\mathrm{a,b}} = \mu_0\, \underline{\underline{I}} , \quad \underline{\underline{\xi}}^{\mathrm{a,b}} = \underline{\underline{\zeta}}^{\mathrm{a,b}} = \underline{\underline{0}} , \tag{9}$$

where ϵ_0 and μ_0 are the permittivity and permeability of free space, $\underline{u}$ is a unit vector parallel to the optical axis of the uniaxial medium, and $\underline{\underline{I}}$ is the 3×3 unit dyadic. The calculated nonzero components of the permittivity dyadic

$$\underline{\underline{\epsilon}}^{\mathrm{HCM}} = \epsilon_0 \left[\epsilon^{\mathrm{HCM}}\, \underline{\underline{I}} + \left(\epsilon_{\mathrm{u}}^{\mathrm{HCM}} - \epsilon^{\mathrm{HCM}} \right) \underline{u}\, \underline{u} \right] , \tag{10}$$

are plotted as functions of f_{b} in Figure 1; trivially, $\underline{\underline{\mu}}^{\mathrm{HCM}} = \mu_0\, \underline{\underline{I}}$, $\underline{\underline{\xi}}^{\mathrm{HCM}} = \underline{\underline{\zeta}}^{\mathrm{HCM}} = \underline{\underline{0}}$. The order of the IMG calculations was set to $N = 5$ to keep the differences with the DMG appreciable on the graphs presented. Both the DMG and IMG estimates are bounded by the MG and the Br estimates for $0 \leq f_{\mathrm{b}} \leq 1$.

We now consider a fully bianisotropic composite medium, *viz.*, a chiroferrite conceptualized as a random deposition of electrically small, isotropic chiral spheres in a ferrite host. The constitutive dyadics are denoted as

$$\underline{\underline{\tau}}^{\alpha} = \tau_0 \left[\tau^{\alpha}\, \underline{\underline{I}} - i \tau_{\mathrm{g}}^{\alpha}\, \underline{u} \times \underline{\underline{I}} + \left(\tau_{\mathrm{u}}^{\alpha} - \tau^{\alpha} \right) \underline{u}\, \underline{u} \right] , \tag{11}$$
$$(\tau = \epsilon,\ \xi,\ \zeta,\ \mu; \quad \alpha = \mathrm{a,\ b,\ MG,\ Br,\ IMG,\ DMG});$$

and we chose the following parameter values: $\epsilon_{\mathrm{u}}^{\mathrm{a}} = \epsilon^{\mathrm{a}} = 5$, $\epsilon_{\mathrm{g}}^{\mathrm{a}} = 0$, $\underline{\underline{\xi}}^{\mathrm{a}} = \underline{\underline{\zeta}}^{\mathrm{a}} = \underline{\underline{0}}$, $\mu_{\mathrm{u}}^{\mathrm{a}} = \mu^{\mathrm{a}} = 1.1$, $\mu_{\mathrm{g}}^{\mathrm{a}} = 1.3$ for medium a; and $\epsilon_{\mathrm{u}}^{\mathrm{b}} = \epsilon^{\mathrm{b}} = 4$, $\epsilon_{\mathrm{g}}^{\mathrm{b}} = 0$, $\underline{\underline{\zeta}}^{\mathrm{b}} = -\underline{\underline{\xi}}^{\mathrm{b}}$, $\xi_{\mathrm{u}}^{\mathrm{b}} = \xi^{\mathrm{b}} = 1$, $\xi_{\mathrm{g}}^{\mathrm{b}} = 0$, $\mu_{\mathrm{u}}^{\mathrm{b}} = \mu^{\mathrm{b}} = 1.5$, $\mu_{\mathrm{g}}^{b} = 0$ for medium b. Estimates of the three nonzero scalar components of the constitutive dyadics $\underline{\underline{\epsilon}}^{\mathrm{HCM}}$, $\underline{\underline{\xi}}^{\mathrm{HCM}}$, and $\underline{\underline{\mu}}^{\mathrm{HCM}}$, are plotted as functions of f_{b} in Figure 2. Results for $\underline{\underline{\zeta}}^{\mathrm{HCM}}$ are not displayed since $\underline{\underline{\xi}}^{\mathrm{HCM}} = -\underline{\underline{\zeta}}^{\mathrm{HCM}}$ follows numerically from all four formalisms.

Clearly, the differences between the predictions of the homogenization formalisms studied here are relatively small. The simplicity and robustness of the numerical implementation is then a clear advantage for the Incremental/Differential Maxwell Garnett formalisms over the Bruggeman formalism.

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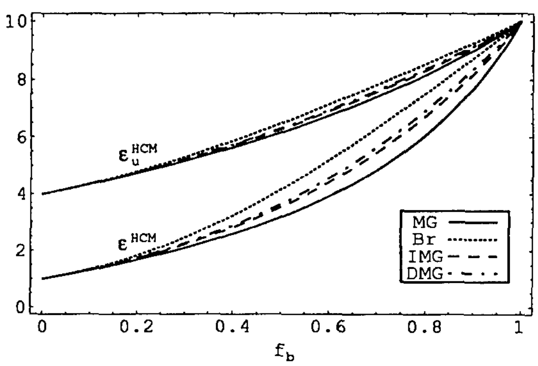

Figure 1: Relative permittivity scalars of a uniaxial dielectric composite as functions of the inclusion volumetric proportion f_b.

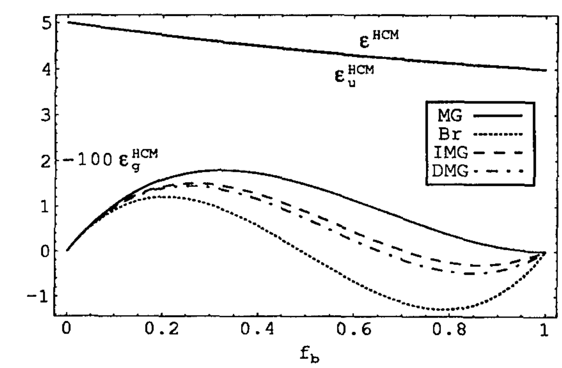

Figure 2a: Constitutive parameters ϵ^{HCM}, $\epsilon_u^{HCM}, \epsilon_g^{HCM}$ of a chiroferrite HCM as functions of the inclusion volumetric proportion f_b.

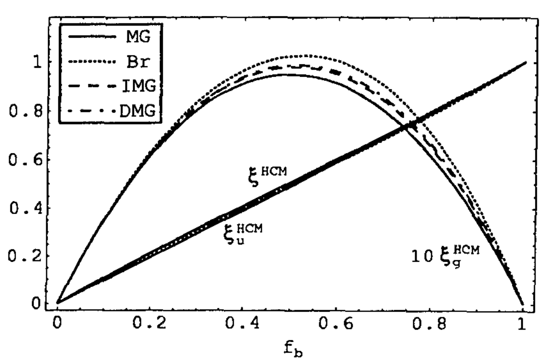

Figure 2b: Constitutive parameters ξ^{HCM}, ξ_u^{HCM}, ξ_g^{HCM} of a chiroferrite HCM as functions of the inclusion volumetric proportion f_b.

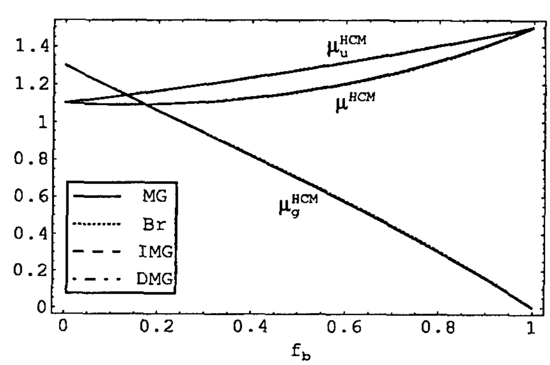

Figure 2c: Constitutive parameters μ^{HCM}, μ_u^{HCM}, μ_g^{HCM} of a chiroferrite HCM as functions of the inclusion volumetric proportion f_b.